Title: Materials Dynamics

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Report
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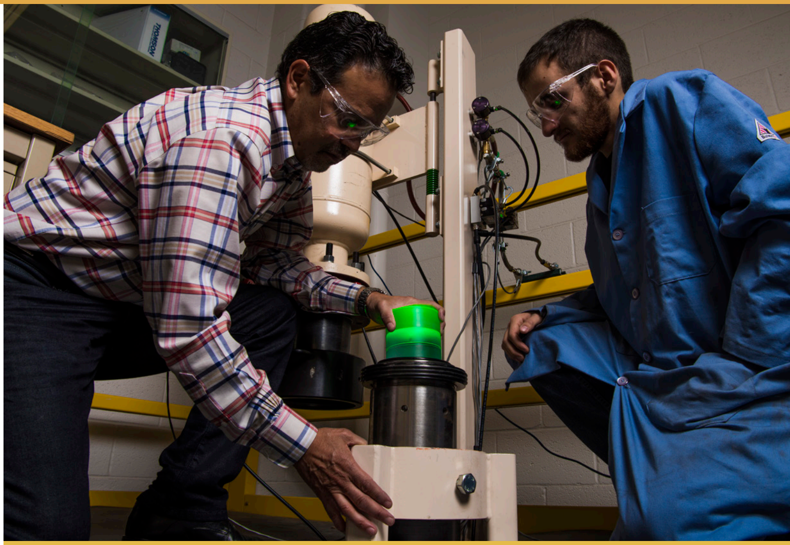
MATERIALS DYNAMICS

The Materials Dynamics area of leadership focuses on understanding structure-properties-performance relationships for the extreme conditions of dynamic loading. This research encompasses controlled synthesis of materials to meet dynamic performance requirements and requires computational coupling across length and time scales for three-dimensional microstructure modeling. For this leadership area, we define dynamic loading as strain rates greater than 10^3/s. A key grand challenge of this area is to predict and measure the evolution of microstructural phases, defect structures, and electronic structure under dynamic conditions while also dynamically measuring local temperature to understand transition states. Solving this challenge will require agile, multidimensional data analysis and interpretation capability.

To solve this grand challenge of understanding the effects of shock loading on material behavior, our approach needs to include:

- experiments designed to explore, quantify, and thereby define the parameters and correlations of importance (shock loading rate, peak shock stress, pulse duration, rarefaction rate, etc.) and their specific effects on various material structure/property relationships;
- rationalization of observations within a systematic framework such as dislocation dynamics or dislocation kinetics coupled with mesoscale material microstructure evolution; and
- modeling based on first principles understanding of all the relevant physics involved.

Increased utilization of first principles modeling solutions beyond the currently used phenomenological models are critically important to future advances in our understanding of shock effects on materials. Future materials research needs to expand from the traditional emphasis of conducting stand-alone x-ray radiography, rear-surface velocimetry, or shock-recovery studies to multidisciplinary investigations of a material's total response. Such investigations would integrate various real-time, in situ experiments, including advanced in situ diagnostics such as proposed for MaRIE, the Laboratory's experimental capability for the study of matter-radiation interactions in extremes, in concert with wave profile data, shock-recovery insights, and theoretical modeling.



Performance prediction of materials subjected to dynamic loading rates is critically important for our national security missions, where materials are often subjected to high explosive drive as well as other dynamic loading conditions. Here, Los Alamos researchers load a 100-mm projectile into a gas gun in preparation for a shock loading experiment on tantalum.

Materials for the Future

The Los Alamos National Laboratory Materials for the Future strategy derives from our vision to support the Laboratory's national security mission drivers.

We pursue the discovery science and engineering for advanced and new materials to intentionally control functionality and predict performance relevant to ensuring the success of the Lab's missions.

To deliver on our missions, our materials strategy builds on materials science and engineering, enabling the necessary Laboratory leadership in seven key areas:

- Complex Functional Materials
- Material Resilience in Harsh Service Conditions
- Manufacturing Science
- Actinides and Correlated Electron Materials
- Integrated Nanomaterials
- Energetic Materials
- Materials Dynamics

Such studies could lend insight, quantify, and clarify some of the long-standing issues of shock-wave deformation in materials, specifically defect generation and storage. Surface diagnostics, such as wave profiles, will help us determine the effect of these defect configurations on the shock response of the material.

Los Alamos Leadership in Materials Dynamics

Performance prediction of materials subjected to dynamic loading rates is critically important for our national security missions, where materials are often subjected to high explosive drive as well as other dynamic loading conditions. Since legacy materials may no longer exist or the manufacturing processes used to make these legacy materials may be unavailable, a thorough understanding of the structure-properties-performance linkages is necessary for the development of new materials or manufacturing processes.

To quantify the structure-properties-performance linkages necessary for a predictive capability, Los Alamos integrates world-class staff in theory and simulation coupled with experts performing small and integrated experiments leveraging the Lab's unique and robust capabilities, in partnership with relevant user and external facilities. Our experimental expertise has a diverse range of dynamic driving tools available at one site. These include gas and powder guns, laser drive, and direct high-explosive loading capability, spanning a wide range of strain rates and peak pressures coupled with novel diagnostics such as photon Doppler velocimetry and thermometry.

Additionally, we have developed novel soft capture mechanisms so that the damage mechanisms of the materials subjected to shock loading can be characterized. Leveraging other national laboratory user facilities, e.g., the Advanced Photon Source at Argonne National Laboratory or the Linac Coherent Light Source at the SLAC National Accelerator Laboratory, material response under dynamic loading can be measured in situ. However, these capabilities are not fully sufficient to meet our requirements of studying bulk response of materials with micron and nanosecond resolution. Additionally, these facilities are not equipped to study classified or hazardous materials. For these classes of experiments we will use or develop unique facilities at Los Alamos, e.g., proton radiography, the Dual-Axis Radiographic Hydrodynamic Test Facility, and MaRIE.

Key Science Questions

- What are the deterministic linkages between processing, structure, properties, and performance?
- What are the relevant length and time scales for defects and interfaces controlling dynamic performance of a material?
- What are the operative dissipative mechanisms far from equilibrium?
- What are the relevant representative volume elements and their sensitivities for the conditions of interest?
- How do we fully develop and implement new diagnostics for direct, in situ observation of dynamic phenomena?

10-year End State

For many applications that subject a material to the extreme environment of dynamic loading, a capability to predict aspects of the performance—such as strength, deformation, and failure—is critical. Furthermore, to move beyond predicting these aspects of performance and toward control of this performance, we must understand and then utilize the deterministic relationships between processing-microstructure-properties and performance under dynamic conditions. Thus, an overarching goal is development of predictive tools to link process to performance under dynamic loading conditions.

The 10-year science goal for the Materials Dynamics area of leadership is the demonstration of a three-dimensional, process-structure-property-performance capability for dynamic strength and damage that incorporates a multi-length scale and age-aware equation of state. This will require a robust and seamless integration of sample manufacturing, characterization (pre- and post-mortem), and dynamic loading coupled with real-time data analytics. The future MaRIE capability will be an integral part of the analytic tool set.

For more information, please see materials.lanl.gov or send email to materials@lanl.gov.

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